Cycloate

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 255 °C

Global applicability domain: Inside

Local applicability domain index: 4.14e-01

Confidence level: 6.09e-01

Nearest Neighbors from the Training Set

Image not found
Ethyl N-butylcarbamate
Measured: 202
Predicted: 193

Image not found
DEET
Measured: 290
Predicted: 284

Image not found
N-Butylacetanilide
Measured: 281
Predicted: 284

Image not found
Acetamide, N-phenyl-N-propyl-(9CI)
Measured: 268
Predicted: 282

Image not found
N,N-Diethyl-p-bromoaniline
Measured: 270
Predicted: 259